Mathematical Modelling and Simulation with Comsol Multiphysics II

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3. Freezing Rotating Waves in Reaction Diffusion Systems

3.1 Rotating waves in reaction diffusion systems

Consider a system of reaction diffusion equations in d space dimensions

$$\begin{aligned} u_t(x,t) &= A\triangle u(x,t) + f(u(x,t)) &&, x\in\mathbb{R}^d,\, t>0,\, d\geqslant 2, \\ u(x,0) &= u_0(x) &&, x\in\mathbb{R}^d,\, t=0, \end{aligned} \tag{1}$$

with diffusion matrix $A\in\mathbb{R}^{m,m}$, nonlinearity $f:\mathbb{R}^m\to\mathbb{R}^m$, initial data $u_0:\mathbb{R}^d\to\mathbb{R}^m$ and solution $u:\mathbb{R}^d\times[0,\infty)\to\mathbb{R}^m$. The operator $\triangle$ denotes the Laplacian given by

$$\triangle u(x) := \sum_{i=1}^{d}\frac{\partial^2 u}{\partial x_i^2}(x),\ x\in\mathbb{R}^d.$$

We are interested in rotating wave solutions of (1): A rotating wave of (1) is a solution $u_\star:\mathbb{R}^d\times[0,\infty)\to\mathbb{R}^m$ of the form

$$u_\star(x,t) = v_\star\left(e^{-tS_\star}(x-x_\star)\right) \quad , x\in\mathbb{R}^d,\, t\geqslant 0, \tag{2}$$

with a time-independent function $v_\star:\mathbb{R}^d\to\mathbb{R}^m$, a skew-symmetric matrix $S_\star\in\mathbb{R}^{d,d}$, i.e. $S_\star^T=-S_\star$, and a vector $x_\star\in\mathbb{R}^d$. The function $v_\star:\mathbb{R}^d\to\mathbb{R}^m$ is called the profile of the rotating wave. The vector $x_\star\in\mathbb{R}^d$ can be considered as the center of rotation for $d=2$ and as the support vector of the axis of rotation for $d=3$. In case $d\in\{2,3\}$, $S_\star\in\mathbb{R}^{d,d}$ can be considered as the angular velocity tensor associated to the angular velocity vector $\omega\in\mathbb{R}^{\frac{d(d-1)}{2}}$ containing $S_\star^{ij}$, $i=1,\ldots,d-1$, $j=i+1,\ldots,d$. Note that the skew-symmetry of $S_\star$ implies that $e^{-tS_\star}$ is a rotation matrix. A rotating wave $u_\star$ is called a localized, if

$$\lim_{|x|\to\infty}|v_\star(x)-v_\infty| = 0 \text{ for some } v_\infty\in\mathbb{R}^m.$$

Our aim is to approximate rotating wave solutions of (1). The idea for approximating the rotating wave $u_\star$ is to determine the profile $v_\star$, the angular velocity tensor $S_\star$ and the vector $x_\star$. This requires to transform (1) into a co-rotating coordinate system.
Transforming (1) via $u(x,t)=v(\xi,t)$ with $\xi:=e^{-tS_\star}(x-x_\star)$ in a co-rotating frame yields

$$\begin{aligned} v_t(\xi,t) &= A\triangle v(\xi,t) + \langle S_\star\xi,\nabla v(\xi,t)\rangle + f(v(\xi,t)) &&, \xi\in\mathbb{R}^d,\, t>0,\, d\geqslant 2, \\ v(\xi,0) &= u_0(\xi) &&, \xi\in\mathbb{R}^d,\, t=0, \end{aligned} \tag{3}$$

where the drift term is defined by

$$\langle S_\star x,\nabla v(x)\rangle := \sum_{i=1}^{d}\sum_{j=1}^{d} S_\star^{ij}x_j D_i v(x), \quad D_i := \frac{\partial}{\partial x_i} \tag{4}$$

In case of skew-symmetric matrices $S_\star=-S_\star^T$, the drift term from (3) is a rotational term containing angular derivatives

$$\langle S_\star x,\nabla v(x)\rangle = \sum_{i=1}^{d-1}\sum_{j=i+1}^{d} S_\star^{ij}\left(x_j D_i - x_i D_j\right)v(x). \tag{5}$$

The operator $A\triangle v(x) + \langle S_\star x, \nabla v(x)\rangle$ is called the Ornstein-Uhlenbeck operator. It is given by the sum of the diffusion term $A\triangle v(x)$ and the drift term $\langle S_\star x, \nabla v(x)\rangle$ and has unbounded (indeed linearly growing) coefficients.
Inserting (2) into (1) shows, that $v_\star$ is a stationary solution of (3), i.e. $v_\star$ solves the rotating wave equation

$$0 = A\triangle v_\star(\xi) + \langle S_\star\xi, \nabla v_\star(\xi)\rangle + f(v_\star(\xi)) \quad, \xi \in \mathbb{R}^d. \tag{6}$$

We are also interested in nonlinear stability of rotating waves. It is well known from the literature, that (at least for $d = 2$) spectral stability implies nonlinear stability. For investigating spectral stability of rotating waves, we must analyze the spectrum of the linearization of the right hand side in (3) at the wave profile $v_\star$, i.e.

$$[\mathcal{L}w](\xi) = A\triangle w(\xi) + \langle S_\star\xi, \nabla w(\xi)\rangle + Df(v_\star(\xi))w(\xi) \quad, \xi \in \mathbb{R}^d.$$

This requires to find solutions (λ, w) with $\lambda \in \mathbb{C}$ and $w : \mathbb{R}^d \to \mathbb{C}^m$ of the eigenvalue problem

$$\lambda w(\xi) = A\triangle w(\xi) + \langle S_\star\xi, \nabla w(\xi)\rangle + Df(v_\star(\xi))w(\xi) \quad, \xi \in \mathbb{R}^d, \tag{7}$$

with eigenfunction $w : \mathbb{R}^d \to \mathbb{C}^m$ and eigenvalue $\lambda \in \mathbb{C}$.
Approximating $v_\star$ via (3) requires the knowledge about the angular velocity tensor $S_\star$ which is in general unknown. This motivates to introduce the freezing method, whose idea is it to approximate the profile $v_\star$, the angular velocity tensor $S_\star$ and the vector $x_\star \in \mathbb{R}^d$ simultaneously.

3.2 Freezing method for rotating waves

Consider again a system of reaction diffusion equations, cf. (1),

$$\begin{aligned} u_t(x,t) &= A\triangle u(x,t) + f(u(x,t)) && , x \in \mathbb{R}^d,\, t > 0,\, d \geqslant 2, \\ u(x,0) &= u_0(x) && , x \in \mathbb{R},\, t = 0. \end{aligned} \tag{8}$$

Introducing new unknowns $\gamma(t) = (R(t), \tau(t)) \in \mathrm{SO}(d) \times \mathbb{R}^d = \mathrm{SE}(d)$ (position) and $v(\xi, t) \in \mathbb{R}^m$ (profile) via the rotating wave ansatz

$$u(x,t) = v(\xi,t),\, \xi := R(t)^{-1}(x - \tau(t)) \quad, x \in \mathbb{R}^d,\, t \geqslant 0, \tag{9}$$

inserting (9) into (8) (the computation will be omitted) and introducing a new unknown $\mu(t) = (S(t), \lambda(t)) \in \mathfrak{so}(d) \times \mathbb{R}^d = \mathfrak{se}(d)$ via $\begin{pmatrix} R_t(t) \\ \tau_t(t) \end{pmatrix} = \begin{pmatrix} R(t)S(t) \\ R(t)\lambda(t) \end{pmatrix}$ yields

$$\begin{aligned} v_t(\xi,t) &= A\triangle v(\xi,t) + \langle S(t)\xi + \lambda(t), \nabla v(\xi,t)\rangle + f(v(\xi,t)) && , \xi \in \mathbb{R}^d,\, t > 0, \\ \begin{pmatrix} R_t(t) \\ \tau_t(t) \end{pmatrix} &= \begin{pmatrix} R(t)S(t) \\ R(t)\lambda(t) \end{pmatrix} && , t > 0. \end{aligned} \tag{10}$$

Equ. (10) has to be equipped with suitable initial data. Requiring $R(0) = I_d$ and $\tau(0) = 0$, (9) and (8) imply

$$v(\xi, 0) = u_0(\xi) \quad, \xi \in \mathbb{R}^d,\, t = 0. \tag{11}$$

Collecting the equations (10), $R(0) = I_d$, $\tau(0) = 0$ and (11) we obtain

$$\begin{aligned} v_t(\xi,t) &= A\triangle v(\xi,t) + \langle S(t)\xi + \lambda(t), \nabla v(\xi,t)\rangle + f(v(\xi,t)) && , \xi \in \mathbb{R}^d,\, t > 0, \\ v(\xi,0) &= u_0(\xi) && , \xi \in \mathbb{R}^d,\, t = 0, \\ \begin{pmatrix} R_t(t) \\ \tau_t(t) \end{pmatrix} &= \begin{pmatrix} R(t)S(t) \\ R(t)\lambda(t) \end{pmatrix} && , t > 0, \\ \begin{pmatrix} R(0) \\ \tau(0) \end{pmatrix} &= \begin{pmatrix} I_d \\ 0 \end{pmatrix} && , t = 0. \end{aligned} \tag{12}$$

(12) contains the equations for v and $\gamma = (R, \tau)$. But so far, the system (12) is not well-posed, since there is still no equation for $\mu = (S, \lambda)$. To determine μ we require an additional algebraic

constraint, a so called phase condition: For this purpose let $\hat{v} : \mathbb{R}^d \to \mathbb{R}^m$ be a template function, e.g. $\hat{v} = u_0$. The idea of the phase condition is to choose $v(\cdot,t)$ such that

$$\min_{g:=(\tilde{R},\tilde{(\tau)})\in \mathrm{SE}(d)} \left\| v(\cdot,t) - \hat{v}(\tilde{R}^{-1}(\cdot - \tilde{\tau}))\right\|^2_{L^2(\mathbb{R}^d,\mathbb{R}^m)} = \|v(\cdot,t) - \hat{v}(\cdot)\|^2_{L^2(\mathbb{R}^d,\mathbb{R}^m)} \quad , t \geqslant 0.$$

A necessary condition to guarantee that the left hand side attains its minimum at $g = (I_d, 0)$ is that the first derivative of $\left\| v(\cdot,t) - \hat{v}(\tilde{R}^{-1}(\cdot - \tilde{\tau}))\right\|^2_{L^2(\mathbb{R}^d,\mathbb{R}^m)}$ evaluated at $g := (\tilde{R}, \tilde{\tau}) = (I_d, 0)$ vanishes, i.e.

$$\begin{aligned} 0 &\overset{!}{=} \left[\frac{d}{d(\tilde{R},\tilde{\tau})}\Big(v(\cdot,t) - \hat{v}(\tilde{R}^{-1}(\cdot-\tilde{\tau})), v(\cdot,t) - \hat{v}(\tilde{R}^{-1}(\cdot-\tilde{\tau}))\Big)_{L^2(\mathbb{R}^d,\mathbb{R}^m)}\right]_{g=0} \\ &= 2\left(v(\cdot,t) - \hat{v}, \left\langle \tilde{S}\cdot + \tilde{\lambda}, \nabla\hat{v}\right\rangle\right)_{L^2(\mathbb{R}^d,\mathbb{R}^m)} \qquad \forall\, (\tilde{S},\tilde{\lambda}) \in \mathfrak{se}(d). \end{aligned} \tag{13}$$

Requiring (13) for every basis element $(I_{ij} - I_{ji}, 0)$ $(i = 1,\ldots,d-1,\ j = i+1,\ldots,d)$ and $(0, e_l)$ $(l = 1,\ldots,d)$ of $\mathfrak{se}(d)$, we obtain for all $t \geqslant 0$

$$\begin{aligned} 0 &= (v(\cdot,t) - \hat{v}, (\xi_j D_i - \xi_i D_j)\hat{v})_{L^2(\mathbb{R}^d,\mathbb{R}^m)} &&, i = 1,\ldots,d-1,\ j = i+1,\ldots,d, \\ 0 &= (v(\cdot,t) - \hat{v}, D_l\hat{v})_{L^2(\mathbb{R}^d,\mathbb{R}^m)} &&, l = 1,\ldots,d. \end{aligned} \tag{14}$$

Combining (12) and (14) yields a partial differential algebraic evolution equation (PDAE)

$$\begin{aligned} v_t(\xi,t) &= A\triangle v(\xi,t) + \langle S(t)\xi + \lambda(t), \nabla v(\xi,t)\rangle + f(v(\xi,t)) &&, \xi \in \mathbb{R}^d,\ t > 0, \\ v(\xi,0) &= u_0(\xi) &&, \xi \in \mathbb{R}^d,\ t = 0, \\ 0 &= (v(\cdot,t) - \hat{v}, (\xi_j D_i - \xi_i D_j)\hat{v})_{L^2(\mathbb{R}^d,\mathbb{R}^m)} &&, t \geqslant 0, \\ 0 &= (v(\cdot,t) - \hat{v}, D_l\hat{v})_{L^2(\mathbb{R}^d,\mathbb{R}^m)} &&, t \geqslant 0, \\ \begin{pmatrix} R_t(t) \\ \tau_t(t) \end{pmatrix} &= \begin{pmatrix} R(t)S(t) \\ R(t)\lambda(t) \end{pmatrix} &&, t > 0, \\ \begin{pmatrix} R(0) \\ \tau(0) \end{pmatrix} &= \begin{pmatrix} I_d \\ 0 \end{pmatrix} &&, t = 0. \end{aligned} \tag{15}$$

The last two equations in (15) for the position $\gamma = (R, \tau)$ are decoupled from the other equations in (15). Therefore, the γ-equation can be solved in a postprocessing step. The γ-equation is called the reconstruction equation for the rotating wave. Since $(v_\star, \mu_\star)$ with $\mu_\star = (S_\star, \lambda_\star)$ satisfy

$$\begin{aligned} 0 &= A\triangle v_\star(\xi) + \langle S_\star\xi + \lambda_\star, \nabla v_\star(\xi)\rangle + f(v_\star(\xi))\ , \xi \in \mathbb{R}^d, \\ 0 &= (v_\star - \hat{v}, (\xi_j D_i - \xi_i D_j)\hat{v})_{L^2(\mathbb{R}^d,\mathbb{R}^m)}\ , 0 = (v_\star - \hat{v}, D_l\hat{v})_{L^2(\mathbb{R}^d,\mathbb{R}^m)}\ , \end{aligned}$$

we expect for stability reasons, that the solution (v, μ, γ) of (15) satisfies

$$v(t) \to v_\star, \quad \mu(t) = (S(t), \lambda(t)) \to \mu_\star = (S_\star, \lambda_\star) \quad \text{as} \quad t \to \infty. \tag{16}$$

As an indicator for the convergence in (16) we check the quantities

$$\|v_t(\cdot,t)\|_{L^2(\mathbb{R}^d,\mathbb{R}^m)} \quad \text{and} \quad |\mu_t(t)| \tag{17}$$

at each time instance t during the computation. In fact, both of these quantities should be small ($\approx 10^{-16}$), since $v_\star$ and $\mu_\star$ do not vary in time.

3.3 Numerical approximation of rotating waves via freezing method

Solving (1), (15) and (7) numerically, requires to truncate these equations to bounded domains. Let $\Omega \subset \mathbb{R}^d$ be a bounded open domain, then (1) must be satisfied for $x \in \Omega$, and equations (15) and (7) for $\xi \in \Omega$. To guarantee the well-posedness of these problems, we must equip the equations with appropriate boundary conditions. Normally, we choose homogeneous Neumann boundary conditions (also known as no-flux boundary conditions), i.e.

$$\frac{\partial u}{\partial \mathrm{n}}(x)=0,\ x\in\partial\Omega,\quad \frac{\partial v}{\partial \mathrm{n}}(\xi)=0,\ \xi\in\partial\Omega.$$

In this context, $\partial\Omega$ denotes the boundary of Ω and $\overline{\Omega}$ the closure of Ω, e.g. $\Omega=B_R(x_0)=\{x\in\mathbb{R}^d\mid |x-x_0|<R\}\subset\mathbb{R}^d$ with $R>0$ and $x_0\in\mathbb{R}^d$ then $\partial\Omega=\partial B_R(x_0)=\{x\in\mathbb{R}^d\mid |x-x_0|=R\}$ and $\overline{\Omega}=\overline{B_R(x_0)}=\{x\in\mathbb{R}^d\mid |x-x_0|\leqslant R\}$. Numerically, we solve the following equations:

Step 1: (Nonfrozen Equation)

$$\begin{aligned}
&u_t(x,t)=A\triangle u(x,t)+f(u(x,t)) && ,\ x\in\Omega,\ t\in(0,T_1],\ d\geqslant 2,\\
&u(x,0)=u_0(x) && ,\ x\in\overline{\Omega},\ t=0,\\
&\frac{\partial u}{\partial \mathrm{n}}(x,t)=0 && ,\ x\in\partial\Omega,\ t\in[0,T_1].
\end{aligned}\tag{18}$$

First, we determine the solution u of (18). The quantities A, f, u_0, Ω and T_1 are given.

Step 2: (Frozen Equation)

$$\begin{aligned}
&v_t(\xi,t)=A\triangle v(\xi,t)+\langle S(t)\xi+\lambda(t),\nabla v(\xi,t)\rangle+f(v(\xi,t)) && ,\ \xi\in\Omega,\ t\in(0,T_2],\\
&v(\xi,0)=v_0(\xi) && ,\ \xi\in\overline{\Omega},\ t=0,\\
&\frac{\partial v}{\partial \mathrm{n}}(x,t)=0 && ,\ \xi\in\partial\Omega,\ t\in[0,T_2],\\
&0=(v(\cdot,t)-\hat{v},(\xi_jD_i-\xi_iD_j)\hat{v})_{L^2(\Omega,\mathbb{R}^m)} && ,\ t\in[0,T_2],\\
&0=(v(\cdot,t)-\hat{v},D_l\hat{v})_{L^2(\Omega,\mathbb{R}^m)} && ,\ t\in[0,T_2],\\
&\begin{pmatrix}R_t(t)\\ \tau_t(t)\end{pmatrix}=\begin{pmatrix}R(t)S(t)\\ R(t)\lambda(t)\end{pmatrix} && ,\ t\in(0,T_2],\\
&\begin{pmatrix}R(0)\\ \tau(0)\end{pmatrix}=\begin{pmatrix}I_d\\ 0\end{pmatrix} && ,\ t=0.
\end{aligned}\tag{19}$$

Then, we determine the solution (v,μ,γ) with $\mu=(S,\lambda)$ and $\gamma=(R,\tau)$ of (19). The quantities A, f, v_0, $\hat{v}$, Ω and T_2 are given. The final time T_2 may be different to the end time T_1 from (18). The template function is often chosen as $\hat{v}(\xi)=u_0(\xi)$ or $\hat{v}(\xi)=u(\xi,T_1)$, where $u(\cdot,T_1)$ denotes the solution of (18) at the end time T_1. Sometimes one must solve (18) to obtain a suitable template function $\hat{v}$. Also the initial data v_0 is often chosen as $v_0(\xi)=u_0(\xi)$ or $v_0(\xi)=u(\xi,T_1)$. The end time T_2 in (19) is often chosen such that the values of the quantities $\|v(\cdot,t)\|_{L^2(\Omega,\mathbb{R}^m)}$ and $|\mu_t(t)|$, cf. (17), are near 10^{-16}.

Step 3: (Eigenvalue Problem)

$$\begin{aligned}
&\lambda w(\xi)=A\triangle w(\xi)+\langle S_\star\xi+\lambda_\star,\nabla w(\xi)\rangle+Df(v_\star(\xi))w(\xi) && ,\ \xi\in\Omega,\\
&\frac{\partial w}{\partial \mathrm{n}}(\xi)=0 && ,\ \xi\in\partial\Omega.
\end{aligned}\tag{20}$$

Finally, we determine (a predescribed number neig of) eigenvalues λ and associated eigenfunctions w of (20). The quantities A, $\mu_\star=(S_\star,\lambda_\star)$, $v_\star$, f, Ω and neig are given. The profile $v_\star$ and the velocity $\mu_\star=(S_\star,\lambda_\star)$ come actually from a simulation, more precisely we set $\mu_\star:=\mu(T_2)$ and $v_\star(\xi):=v(\xi,T_2)$, where $\mu(T_2)$ and $v(\cdot,T_2)$ denote two components of the solution of (19) at the end time T_2.